

RESOURCES IN PLASMA SPECTROSCOPY

- CURRENT TECHNOLOGIES @ IAEA

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International Atomic Energy Agency (IAEA)

<http://www.iaea.org/>

- Founded in 29 July 1957
- Vienna, Austria
- 171 Member States (5 Feb 2019)
- 6 departments
- 2500 workers
- Regular budget €364M
- 144 countries receiving support through technical cooperation
- assists its Member States, in the context of social and economic goals, in planning for and using nuclear science and technology for various peaceful purposes, including the generation of electricity, and facilitates the transfer of such technology and knowledge in a sustainable manner to developing Member States;



IAEA

• 500 000 visitors/month to [iaea.org](http://www.iaea.org)

IAEA Atomic and Molecular Data Unit

Fusion research requires huge amounts of material data – AM/PSI data

- IAEA A+M Unit formed in 1977
 - Under the supervision of International Fusion Research Council (IFRC) subcommittee on atomic, molecular and plasma-surface interaction data.
 - A+M Unit part of Nuclear Data Section (<https://www-nds.iaea.org/>)
- Review progress and achievements of Atomic, molecular and plasma-surface interaction (A+M/PSI) data for Fusion programme
- Stimulate international cooperation in measurement, compilation and evaluation of A+M / PSI data for fusion

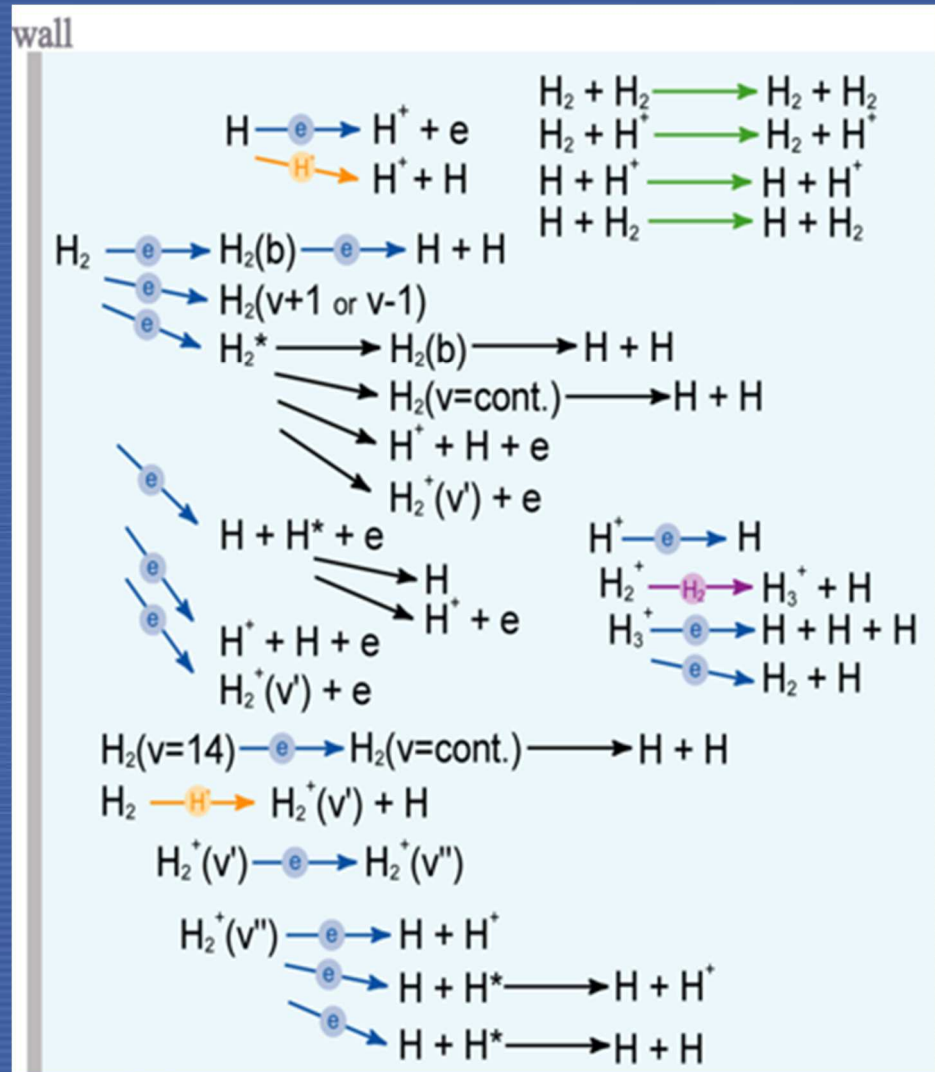
Unit Head: Christian Hill

Atomic Physicist: Kalle Heinola

Scientific Data Manager: Ludmila Marian

A+M Data Unit priorities

Example of atomic and molecular processes required for Hydrogen



Atomic data

D, T, He, Be, C, O, N, Ne, W, Xe, Kr, Ar
Ti, Cr, Fe, Cl, Mo, V, Cu, Li, Sn, B, S, Cs,
Hf, Ta

Excitation, Ionization, Recombination
Charge exchange

Molecular data

H_2 , H_2^* , H_2^+ , H_3^+ , H_2O , CO , CO_2 , CH_4 , CH ,
 C_2 , Be hydrides, oxides and nitrides, N_2 ,
and other hydrocarbons and radicals
including hydrogen isotopic variants
B, LiH, SnH_4 , Cs hydrides and oxides

Excitation, Ionization, Recombination,
Dissociation

Plasma-Surface Interaction data

D, T, He, Be, C, O, N, Ne, W, Xe, Ar,
Be-W, Be-O, W-O, Be-C, C-W, Be-C-W


Sputtering, Reflection, Penetration,
Adsorption, Gettering, Diffusivity

A+M Data Unit

interim url

<https://www-amdis.org/>

<https://www-amdis.org/>



International Atomic Energy Agency
Atomic Molecular Data
Provided by the Nuclear Data Section

Databases » AMBDAS | ALADDIN | OPEN-ADAS

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Atomic and Molecular Data

The Atomic and Molecular Data Unit is to establish and maintain a solid surface interaction process

Databases on Atomic and Molecular Data

Atom, Molecule
Plasma-Surface
Data

ALADDIN
Numerical
Database

Online Computing Capabilities

Code
Centres
Portal

LANL
Atomic
Physics

Knowledge Base for Atomic and Molecular Data

Our Unit achieves its objective of international **Coordinated Research** (research contracts, research interaction (PMI) data inform

The activity of Our Unit is supported by the

IAEA Nuclear Data Section



IAEA-NDS
Mission, Staff Nuclear Data
and more



Nuclear
Services



Meetings
Workshops

AMD Unit | **About** | Activities | Databases | Online Computing

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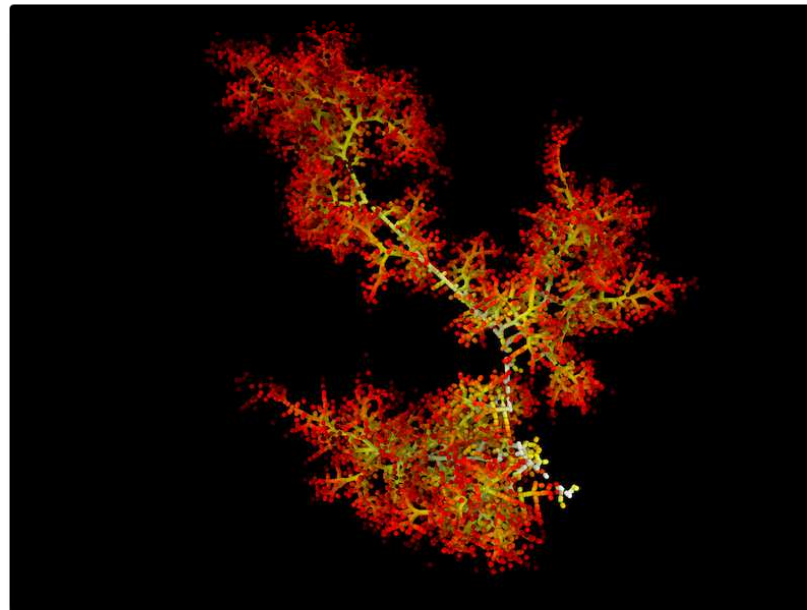
The Atomic and Molecular Data Unit establishes and maintains numerical databases of fundamental data for fusion energy research, and facilitates collaborative international research in the production and evaluation of such data. [Read more.](#)

Recent and Upcoming Meetings

| | |
|-----------------|---|
| 6 – 10 May 2019 | ICTP Workshop 2019: Atomic and Molecular Spectroscopy in Plasmas |
| 6 – 7 June 2019 | Consultancy Meeting on Evaluation of Fundamental Data on Beryllium-containing Species for Edge Plasma Modelling |

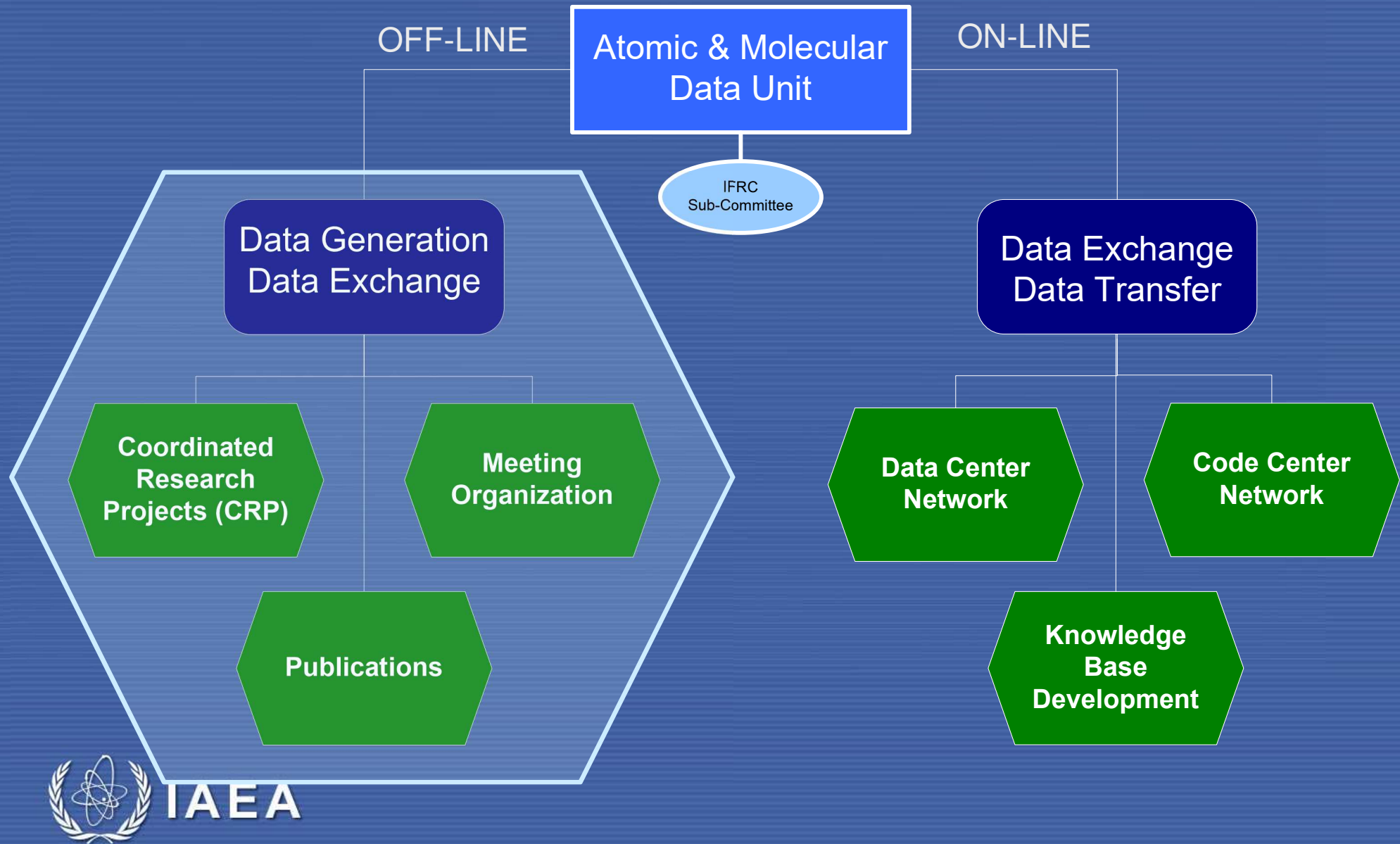
Quick Links

- Our CRPs
 - Hydrogen Permeation (planned)
 - Vapour Shielding
 - Neutral Beams
 - Steel Surfaces
 - Irradiated Tungsten
- Our Meetings
- Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP)
- Conferences and workshops in atomic and molecular physics



An illustration of the simulated collisional cascade in tungsten caused by the impact of a 200 keV neutron.

Overview of A+M Data Unit Activities



Coordinated Research Projects (CRP)

Data Generation and Exchange

CRP: Coordinated Research Project

- Main mechanism by which the AMD Unit encourages new research
- Unique opportunity for comprehensive and synergistic collaboration

Joint research on A+M and PSI data for fusion

- Representatives from 10 to 15 institutes worldwide
- Duration 3 – 4 years; 3 Research Coordination Meetings (RCM)

Objectives: to define and coordinate international research on

- Generation, compilation, and evaluation of data
- Establishment of databases
- Development of new techniques

Outputs:

- Publications, Meeting presentations and reports
- Final reports historically “Atomic and Plasma-material Interaction Data for Fusion (APID)”; more recently in journals (JPCF, Atoms, Nuclear Fusion)
- Data and results in ALADDIN numerical Database and Knowledge Base

Coordinated Research Projects (CRP)

Data Generation and Exchange

Up-to-date list on interim url <https://www-amdis.org/CRP/>

(<https://www-amdis.org/> → Activities → CRPs)

AMD Unit | About | Activities | Databases | Online Computing

CRPs | Data Centres Network | Code Centres Network | GNAMPP | Meetings | Workshops

Coordinated Research Projects

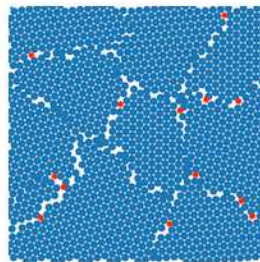
Coordinated Research Projects (CRPs) bring together scientists representing institutes in Member States to collaborate on a focussed research topic that is of shared interest and is important to the mission of the Agency. A CRP is normally approved for a period of 3–5 years and involves 8–15 laboratories, research teams or institutions. Most CRPs involve three Research Coordination Meetings (RCMs) where participants are brought together. The IAEA supports the cost of the RCMs, but only very limited funds are available for direct research support, and this only for participants from developing countries.

In the case of CRPs organized by the AMD Unit, the goals of the CRP may include the establishment of a particular database, data generation, compilation and assessment for specific types of atomic and molecular collision processes. A CRP generally results in a significant amount of new data on collision processes or structural properties of elements or materials relevant to fusion energy research. In addition a CRP may provide detailed critical assessments of the existing data and selection of sets of data that are recommended as the best available at the time of the assessment. The CRP results of adequate accuracy and completeness are stored in the ALADDIN database and published in the IAEA publication series Atomic and Plasma-Material Interaction Data for Fusion (APID).

During the last 10 years the IAEA AMD Unit has been running about an average of about three active CRPs at a time.

Planned CRPs

Hydrogen Permeation in Nuclear Materials



This proposed CRP is at an early stage of planning. It will seek to enhance the knowledge base and reduce uncertainties in data concerning the migration of hydrogen in materials of relevance to nuclear fusion reactors. Of primary interest are candidate divertor and first-wall materials such as tungsten and various types of reduced-activation ferritic/martensitic steel (RAFM), but various copper alloys, as well as materials used in the nuclear fission industry may also be in scope.

[Full details](#)

Active CRPs

Atomic Data for Vapour Shielding in Fusion Devices

Meetings, Workshops

Data Generation and Exchange

<https://www-amdis.org/meetings/>

<https://www-amdis.org/> → Activities → Meetings
→ Workshops

AMD Unit | [About](#) [Activities](#) [Databases](#) [Online Computing](#)

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Meetings

The IAEA AMD Unit organizes several types of experts' meetings:

- *Technical Meetings (TMs)* of experts with a broad spectrum of expertise to provide advice regarding either general policy and programme orientation questions, or on specific technical issues concerning Unit's activity;
- *Consultants' Meetings (CMs)* of experts to obtain advice or perform a specific task related to a particular database or activity;
- *Research Coordination Meetings (RCMs)* are meetings of the Principal Scientific Investigators representing groups participating in a [Coordinated Research Projects](#) (see CRPs).

These meetings differ in the allowed number of participants and the level of Agency support for participants. IAEA AMD Unit organizes, on average, 4 – 6 experts' meetings each year. The proceedings and the results are described in a Summary Report issued shortly after the meeting.

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[ICTP Workshops](#)

[Other Workshops](#)

ICTP Workshops

The IAEA organizes several Workshops in conjunction with the [Abdus Salam International Centre for Theoretical Physics \(ICTP\)](#) in Trieste; in recent years the AMD Unit has participated in this by running an annual event to provide training and information exchange for computational scientists working on models and data for atomic, molecular and materials processes relevant to fusion energy research.

The workshops are aimed at advanced PhD students and other early-stage career researchers, particularly those from developing countries.

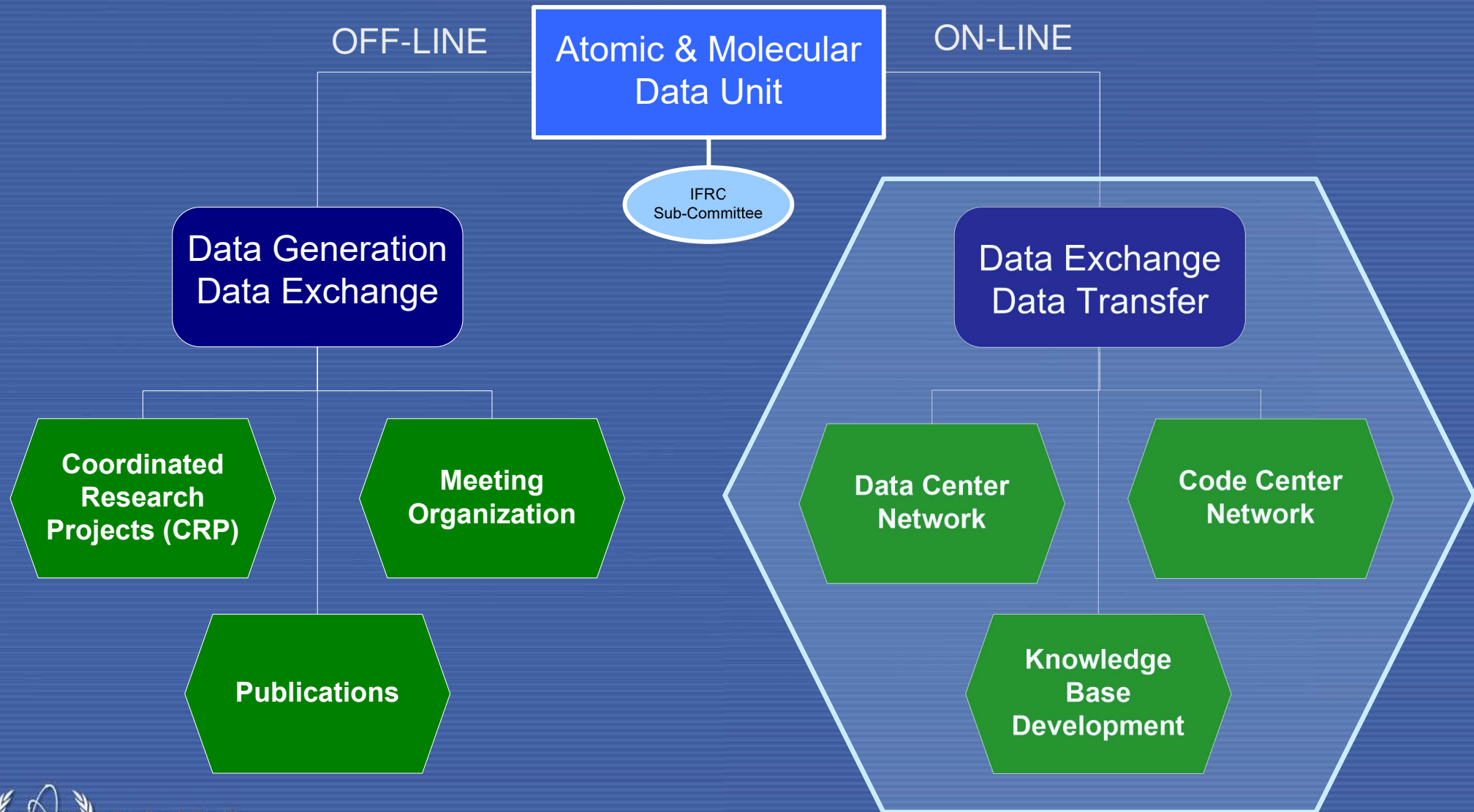
ICTP Workshop 2020: Radiation Damage in Nuclear Systems: from Bohr to Young

This proposed Workshop will assist Ph.D. students and early-career researchers develop a quantitative understanding of the impact of radiation damage on materials, both for existing fission and proposed fusion reactors. There is an emphasis on the conceptual progression of theoretical and experimental techniques across spatial scales from atomistic descriptions to the macroscopic behaviour of bulk material.

[Full details](#)



Overview of A+M Data Unit Activities



Data Centre Network (DCN) activities

Data Exchange and Transfer

Domain : A+M and PSI data as well as bulk material properties (plasma-material interaction - PMI) data for fusion and other applications.

(A+M/PSI/PMI)

Established Program: Collection, Dissemination, Critical assessment (evaluation) and generation of A+M, PSI, and PMI data

- ALADDIN: Numerical Database (A+M/PSI)
- AMBDAS: Bibliographic Database
- CASCADESDB: Irradiations damage Database (PMI)
- CLERVAL: Events and Institutes Database
- OPEN-ADAS: Numerical Database
- GENIE: Search Engine on Numerical Databases

Data Centre Network (DCN) activities

Data Exchange and Transfer

<https://www-amdis.org/databases/>

AMD Unit | [About](#) [Activities](#) [Databases](#) [Online Computing](#)

Databases

The Atomic and Molecular Data Unit manages several numerical and bibliographic databases for fusion and other plasma science research:

[AMBDAS](#): Atomic and Molecular Bibliographic Data System

[ALADDIN](#): Numerical database of collisional cross sections and plasma-material interaction data

[CascadesDB](#): Database of Molecular Dynamics simulations of collision cascades in materials of relevant to fusion research

[Clerval](#): Database of institutions, people and events related to atomic and molecular data

Further resources

ORNL "Red Book" Series: Atomic Data for Fusion

The Controlled Fusion Atomic Data Center (CFADC) at Oak Ridge National Laboratory (ORNL) produced a series of printed compilations of atomic data for fusion applications known as the "Red Books". Since its closure, scanned versions of some of these reports have been difficult to find – they are provided for download below as a convenience to the fusion data community.

- [Volume 1: "Collisions of H, H₂, He and Li Atoms and Ions with Atoms and Molecules"](#) (pdf: 10.8 MB), C. F. Barnett (ed.), ORNL-6086 (1990)
- [Volume 2: "Collisions of Electrons with Atoms and Molecules"](#), J. W. Gallagher (ed.), ORNL-6087, 2nd ed., (1994)
- [Volume 3: "Atomic Data for Fusion: Particle Interactions with Surfaces"](#) (pdf: 11.4 MB), E. W. Thomas (ed.), ORNL-6088 (1985)



Data Centre Network (DCN) activities

Data Exchange and Transfer

<https://www-amdis.org/databases/>

ALADDIN: Numerical database

- Atomic and Molecular collisional database
 - Heavy particle collisions / electron collisions / photon collisions
 - search by reactants, products, process, data types, author, publication
- Plasma-surface interaction database
 - Reflection / sputtering / radiation enhanced sublimation / penetration
 - Search by projectile, surface, chemical component, data type, author, publication
- Data developed through CRPs, and meetings recommended by IFRC

Data Centre Network (DCN) activities

Data Exchange and Transfer

<https://www-amdis.org/databases/>

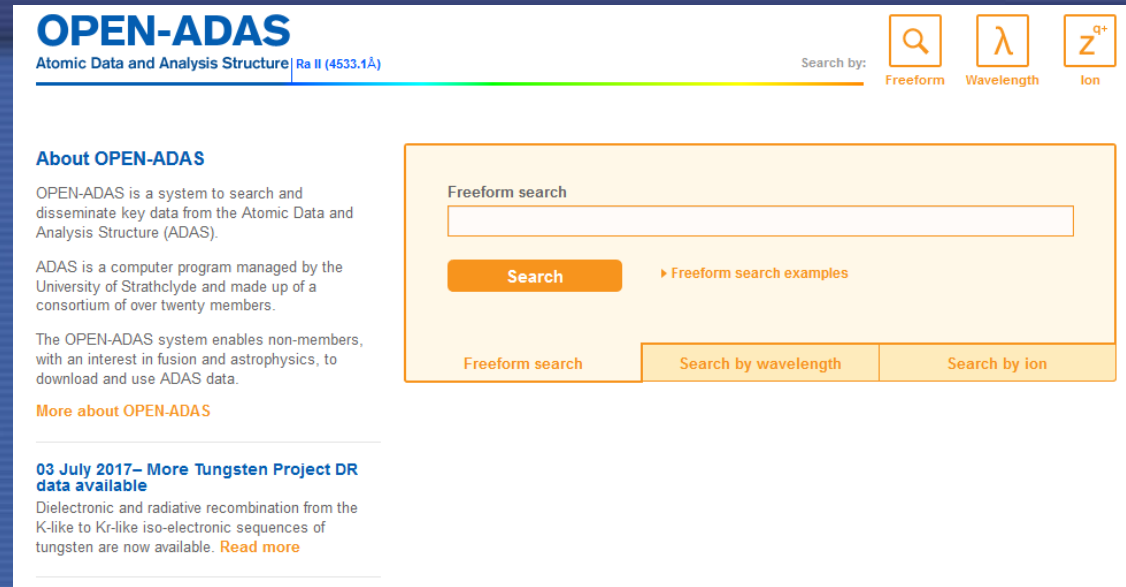
AMBDAS: Bibliographical database

- Data source
 - Spectroscopic data from NIST
 - Collisional data from ORNL
 - Data entries relevant for fusion
- Data search
 - Reactants, processes, authors, keywords, year
 - Results with authors, title, reference and DOI (Digital Object Identifier)

Data Centre Network (DCN) activities

Data Exchange and Transfer

<http://open.adas.ac.uk/>



The screenshot shows the OPEN-ADAS website. At the top, the header includes the text "OPEN-ADAS" and "Atomic Data and Analysis Structure | Ra II (4533.1Å)". To the right of the header are three search icons: a magnifying glass labeled "Search by:", a wavelength symbol (λ) labeled "Wavelength", and an ion symbol (Z^{q+}) labeled "Ion". Below the header, the left column contains an "About OPEN-ADAS" section with descriptive text and a "More about OPEN-ADAS" link. The right column features a "Freeform search" section with a text input field, a "Search" button, and a link to "Freeform search examples". Below this are three tabs: "Freeform search", "Search by wavelength", and "Search by ion". At the bottom of the left column, there is a news item dated "03 July 2017" titled "More Tungsten Project DR data available" with a "Read more" link.


- **ADAS** is an interconnected set of computer codes and data collections for modelling
 - Radiating properties of ions and atoms in plasmas for fusion and astrophysical application
 - Analysis and interpretation of spectral measurements collisional database
- **OPEN-ADAS** is a free web access to ADAS data
 - A joint development between the ADAS Project and the IAEA to provide access to fundamental and derived atomic data from the **ADAS** project and its related databases.

Data Centre Network (DCN) activities

Data Exchange and Transfer

<https://www-amdis.iaea.org/GENIE/>

GENIE
A General Internet Search Engine for Atomic Data

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value="?"/></td></tr><tr><td>MCHF/MCDHF Collection</td><td><input checked="" type="checkbox"/></td><td><input data-bbox="981 807 1003 823" type="button" value="?"/></td></tr><tr><td>KAERI AMODS Spectral Lines</td><td><input checked="" type="checkbox"/></td><td><input data-bbox="981 831 1003 847" type="button" value="?"/></td></tr><tr><td>CAMBD Atomic Spectra</td><td><input checked="" type="checkbox"/></td><td><input data-bbox="981 855 1003 871" type="button" value="?"/></td></tr><tr><td>Spectr-W3</td><td><input checked="" type="checkbox"/></td><td><input data-bbox="981 879 1003 895" type="button" value="?"/></td></tr></table> <p><input type="button" value="Go for A/E/lambda"/> <input type="button" value="Reset"/></p> | NIST Atomic Spectra Database | <input checked="" type="checkbox"/> | <input data-bbox="981 687 1003 703" type="button" value="?"/> | Kurucz's CD-ROM 23 | <input checked="" type="checkbox"/> | <input data-bbox="981 711 1003 727" type="button" value="?"/> | Atomic Line 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<table><tr><td><input checked="" type="radio"/> Excitation <input type="radio"/> Ionization <input type="radio"/> Dielectronic recombination</td><td><input data-bbox="1809 584 1832 600" type="button" value="?"/> Cross sections <input checked="" type="checkbox"/> Rate coefficients <input checked="" type="checkbox"/></td></tr></table> <table><tr><td>IAEA ALADDIN Database</td><td><input checked="" type="checkbox"/></td><td><input data-bbox="1787 679 1809 695" type="button" value="?"/></td></tr><tr><td>NIFS AMDIS Database</td><td><input checked="" type="checkbox"/></td><td><input data-bbox="1787 703 1809 719" type="button" value="?"/></td></tr><tr><td>CAMBD Collisional Processes</td><td><input checked="" type="checkbox"/></td><td><input data-bbox="1787 727 1809 743" type="button" value="?"/></td></tr><tr><td>NIST Atomic Cross Sections</td><td><input checked="" type="checkbox"/></td><td><input data-bbox="1787 751 1809 767" type="button" value="?"/></td></tr><tr><td>OPEN-ADAS</td><td><input 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Web search engine for atomic data

Radiative properties – search on 8 databases

Collisional databases – search on 4 databases

Code Centre Network (CCN) activities

Data Exchange and Transfer

CCN: Joint effort to gather and provide access to any information relevant for modellers in fusion plasma science

- Online computing
 - Downloadable codes
 - Direct contacts with the CCN for any expertise
-
- Online codes for Heavy Particle Collisions
 - Online codes for Average Approximation
 - Online codes for Rate Coefficients
 - Results and link to Los Alamos atomic physics codes
 - Results and link to FLYCHK code

Code Centre Network (CCN) activities

Data Exchange and Transfer

<https://www-amdis.org/online-computing/>

AMD Unit

About Activities Databases Online Computing

Online Computing

Below are some links to online computing resources for calculating plasma properties.

HEAVY: Cross sections for excitation and charge transfer for collisions between hydrogenic targets and bare ions.

AAEXCITE: An interface to average approximation cross sections for calculating electron impact cross sections for atomic ions.

RATES: Results from collisional radiative calculations of plasmas carried out with the Los Alamos modeling codes are available. Interpolations allow the user to obtain total radiated power, average ion charge, and relative ionization populations in a steady state plasma.

(This resource is currently unavailable.)

LANL: An interface is available to run several Los Alamos atomic physics codes for calculation of atomic structure, electron impact excitation, as well as ionization processes. Since 2010, atomic data sets of argon, chlorine and silicon produced by a group at LANL can be downloaded for all ionization stages.

FLYCHK: An interface to the FLYCHK code available at NIST, which generates atomic level populations and charge state distributions for low-Z to mid-Z elements under NLTE(Non-Local Thermodynamic Equilibrium) conditions.

FAC (Flexible Atomic Code): A complete set of collisional and radiative data of atoms from Z=2 (Helium) to Z=14(Silicon).




Knowledge Base and Clerval

Knowledge Base organization (<https://www-amdis.iaea.org/w>)

- Use of Wiki pages – AMD Unit in a coordinator role
- Community ownership: voluntary content contribution & peer review
- Central location – direct data storage or link to data storage
- Provide information on data and their applications in a context
- Closer community network → Foster collaboration on a focused topic

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Main Page

Knowledge Base for Atomic, Molecular and Plasma-Material Interaction Data For Fusion

Introduction

Atomic, molecular and plasma-material interaction processes play an important role in the energy balance, confinement and stability of a thermonuclear plasma. The primary goal of this Knowledge base is to identify the needs in the atomic, molecular and plasma-surface interaction data sets for fusion research, both [magnetic confinement fusion](#) and [inertial confinement fusion studies](#), to provide a direct link to the relevant data sources and present more information on the available data sets.

Data Needs

Magnetic Confinement Fusion

- Introduction
- Spectroscopic Data
- Collisional Data for Edge Studies
- Collisional Data for Neutral-Beam Heating
- Radiative Plasma Cooling
- Plasma-Wall Interaction
- Material Properties

Atomic Data

- Atom-Electron Collisions
- Atom-Heavy-particle Collisions
- Atomic Radiative Properties

Molecular Data

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 - 5.4 Meetings on A+M+PM/PSI Processes and Data
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 - 5.6 European Fusion Development Agreement (EFDA)
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Clerval (<https://www-amdis.org/clerval/>)

- Database of
 - events
 - institutes

relevance to the use, calculation and measurement of
A+M/PSI/PMI data in nuclear fusion research

Knowledge Base and Clerval

Clerval (<https://www-amdis.org/clerval/>)

AMD Unit

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Events

2019

May 2019

| Date | Event |
|-------------|--|
| 19 – 24 May | <p>International Conference on Nuclear Data for Science and Technology (ND 2019), China National Convention Center, Beijing, China</p> <p>Co-organized by OECD-NEA and IAEA</p> <div><div>Atomic Spectroscopy</div><div>Collisions in Plasmas</div><div>Fusion</div><div>Industrial Plasmas</div><div>Plasma Diagnostics</div><div>Plasma–Material Interaction</div></div> |
| 21 – 24 May | <p>17th International Conference on Plasma-Facing Materials and Components for Fusion Applications (PFMC 2019), Eindhoven, Netherlands</p> <p>Dutch Institute for Fundamental Energy Research (DIFFER)</p> <p>Contact: Thomas MORGAN</p> <div><div>Erosion</div><div>Experimental</div><div>Fusion</div><div>ITER</div><div>Liquid Metal Walls</div><div>Plasma–Material Interaction</div><div>Radiation Damage</div><div>Steel</div></div> |



Global Network for the Atomic and Molecular Physics of Plasmas GNAMPP

<https://www-amdis.org/GNAMPP>

Purpose

- Consortium of research groups working in the area of *fundamental A+M* physics relevant to plasma processes
- Focus on promoting *collaboration and communication* between experimentalists and theorists to improve the quality and completeness of data used in modelling and interpreting fusion plasmas

Global Network for the Atomic and Molecular Physics of Plasmas GNAMPP

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Functions

- Data evaluation
- Data dissemination
- Benchmarking calculations against experiments
- Find collaborators
- Setting priorities for data needs in nuclear fusion research
- Mailing list for communicating events, funding, and job opportunities, new data
- Description of research interests with recent publications

GNAMPP

Researcher network

Global Network for the Atomic and Molecular Physics of Plasmas GNAMPP

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